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This is the Accepted version of the following publication

Ghiji, Mohammadmahdi, Goldsworthy, L, Brandner, PA, Garaniya, V and Hield, P (2016) Numerical and experimental investigation of early stage diesel sprays. *Fuel*, 175. 274 - 286. ISSN 0016-2361

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# Numerical and Experimental Investigation of Early Stage Diesel Sprays

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## Abstract

Experimental and numerical investigations of primary atomization in a high-pressure diesel jet are presented. Information on flow processes and structures inside and near nozzle exit are described at early and quasi-steady stages of injection. The numerical method is based on the Volume Of Fluid (VOF) phase-fraction interface capturing technique, in an Eulerian framework. The influence of grid resolution, convection interpolation scheme and temporal integration scheme on the modelling of jet physics are investigated. The present flow setup includes in-nozzle disturbances with the no-slip condition at the walls. All experimental operating conditions are replicated in the numerical models. The early stage liquid jet leading edge demonstrates an umbrella-shaped structure in the numerical results which is in qualitative agreement with experimental imaging. Data obtained provide insight into the flow behavior in the dense region including commencement of fragmentation and early spray angle formation. Experimental images show a cloud of air-fuel mixture at the early stage of injection. The existence of ingested air inside the injector after needle closure could be the source of the observed deviation between experimental and numerical results. The results show that the jet break-up rate and liquid core length increase in cases with higher grid resolutions. The early spray angle from the numerical results at the quasi-steady stage, shows good agreement with experimental data.

## Keywords

High-pressure diesel spray; Primary atomization; Near-nozzle flow; In-nozzle turbulence; Large Eddy Simulation; Eulerian/VOF.

## 1. Introduction

Steady and unsteady liquid jet flows and their breakup remain an ongoing field of investigation [1-8]. Jets are of broad interest for the study of many basic phenomena and in a range of physical processes. They occur at length scales ranging from the order of atomic to that of the universe. In many applications, they may be multi-phase and involve multiple phase changes, chemical reactions and complex flow phenomena.

Human impacts on the environment and more specifically global warming are increasing government concerns on strict emission standards for engine manufacturers. The quality of air-fuel mixing is mainly driven by atomization of the injected liquid jet, which plays an important role in the combustion process, ultimately controlling production of pollutants. Engine manufacturers are constantly aiming to reduce exhaust gas emissions by optimizing the fuel injection process. A wide range of engine operating conditions makes the optimization of air-fuel mixing difficult [8-11]. The motivation, on one hand, is practical applications such as manufacturing of diesel engine injectors and, on the other hand, understanding the origin of key phenomena of atomization and its influence on jet breakup processes.

In diesel engines, combustion chambers are fed by high-pressure fuel injected as a solid cone spray. This spray undergoes a series of instabilities (longitudinal and transverse) which lead to the fragmentation of the liquid bulk into structures that further disintegrate into droplets. This initial process of atomization is called primary breakup and occurs in the vicinity of the injection point. Primary breakup mechanisms initiate the atomization process, control the extent of the liquid core and provide initial conditions for secondary breakup in the disperse flow region [5, 10, 12, 13].

Despite the fact that atomization is widely utilized and significantly affects engine combustion processes, heat release rate and exhaust emissions [2, 14-17], the characteristics of the spray produced

46 (for example size and velocity distributions of droplets) are still not well predicted due to the small length  
47 and time scales and high liquid fractions involved, especially inside the jet.

48 So far, many theories have been proposed to describe the primary atomization mechanism, including:  
49 aerodynamic shear forces which act through stripping and Kelvin-Helmholtz (K-H) instabilities [8, 18,  
50 19]. Turbulence-induced disintegration has a significant effect on jet breakup at higher Reynolds numbers  
51  $Re_l = \rho_l U D / \mu_l$ , where  $\rho_l$  is the liquid density,  $U$  is the liquid velocity,  $D$  is the orifice diameter, and  $\mu_l$  is  
52 the dynamic viscosity [14, 16, 20-23]. Relaxation of the velocity profile, creates a bursting effect  
53 especially in non-cavitating jets and large velocity differentials [24]. Cavitation-induces disintegration of  
54 the jet due to the reduction of cross-sectional area at the nozzle inlet [25-28]; and liquid bulk oscillation  
55 provoking toroidal surface perturbations [8, 29].

56 Less of a consensus has been achieved in determining the dominant mechanisms of early breakup  
57 when a high-speed liquid jet is injected into a pressurized dense gas. Many interdependent phenomena  
58 can provoke severe velocity fluctuations leading to a nonlinear instability of the flow inside the nozzle.  
59 These phenomena include turbulence [16, 20-23] generated by the nozzle geometry and by the collapse of  
60 cavitating bubbles [25-28]. In addition to turbulence, fluctuations of the injection velocity [24] and drop  
61 shedding [14, 30] contribute to the primary breakup. Experimentally separating and investigating these  
62 different effects is very difficult. For the development of diesel engines with both optimal fuel economy  
63 and minimum pollutant emissions, it is necessary to comprehend the spray processes and then  
64 characterize the effects of different parameters and engine operating condition on fuel flow structures.  
65 This is a challenging subject to study, both experimentally and numerically [4, 15, 18, 31, 32]. In this  
66 study, the flow inside the nozzle and the liquid bulk near the nozzle exit and its fragmentation (primary  
67 atomization) are investigated.

This paper concentrates on the effect of in-nozzle turbulence. The effects of cavitation will be studied in future work. Turbulent flows are represented by eddies with an entire range of length and time scales. Large eddy simulation (LES) directly resolves large scale eddies and models small eddies. Simulating only small eddies and solving the large eddies allows the use of much coarser meshes and longer time steps in LES compared to Direct Numerical Simulation (DNS). Despite this, LES still needs principally finer meshes compared to the ones used for Reynolds Averaged Navier Stokes (RANS) computations. Since RANS models cannot capture the transient spray structure [5, 6, 8, 9] including droplet clustering and shot to shot variability, LES is applied to overcome these limitations.

Literature reviews of the existing atomization models, demonstrated that all these models (blob, Huh/Gosman, MPI, Arcoumanis, Nishimura, V.Berg, Baumgarten, ReitzWave model, Taylor Analogy Breakup model) [9, 32, 33] simplify droplet generation in the dense region (primary atomization) which might make the simulation inaccurate and unrealistic [6, 18]. For example, the blob model as the most employed model not only simply generates parcels with the size of the nozzle diameter but also does not take into account the physics of in-nozzle turbulence and in-nozzle cavitation. In addition, these conventional atomization models with Lagrangian Particle Tracking (LPT), limit the grid fineness near the nozzle and do not allow LES to capture the features of the spray and background fluid flow near the nozzle. Furthermore, refining the grid with the blob method results in problems with high liquid fraction in the LPT approach (too much liquid in each cell) [5, 6, 9, 34]. These limitations motivate the use of the Eulerian approach to model the primary atomization, instead of using conventional atomization models. With ever increasing computational power, there is an incentive to use more complex models for primary atomization. This is a key aim of the present work.

To date, considerable progress has been made in the development of rigorous numerical methods for performing highly resolved simulations of multiphase flow [8, 35]. The accuracy of different numerical techniques for modelling the primary atomization of a liquid diesel jet was investigated in detail for low

Re ( $Re < 5000$ ) by Herrmann [20] and Desjardins & Pitsch [36]. Herrmann [20], demonstrated the importance of the grid resolution on capturing the accurate phase interface geometry of diesel liquid with an injection velocity of 100 m / s and  $Re = 5000$ . Turbulence was reported as the dominant driving mechanism of atomization within the first 20 nozzle diameters downstream.

Due to the lack of detailed studies of the primary atomization of diesel liquid jets under real diesel engine operating conditions, the present study focuses on the structure of primary atomization with an accelerating injection pressure up to 1200 bar, background pressure of 30 bar, liquid Reynolds number within the range  $7000 \leq Re_l \leq 37000$ , and liquid Weber number of  $We_l \approx 933843$  at quasi-steady stage. The liquid Weber number  $We_l = \rho_l U_p d / \sigma$ , where  $U_p$  is the droplet relative velocity,  $d$  is the droplet diameter and  $\sigma$  is the surface tension. The Reynolds number is calculated based on average liquid velocity at the nozzle hole exit. The large range of  $Re$  is due to rising pressure at the sac inlet, changing from 30 bar at the beginning of injection up to 1200 bar at the quasi-steady stage of injection. In-nozzle cavitation is not considered in this work however this constraint will be eliminated in further studies. The present work focuses on the very early stages of injection as it is likely that instabilities generated in the early stages have significant effect on the development of the whole spray. Non-evaporating conditions are employed to simplify the physical complexities.

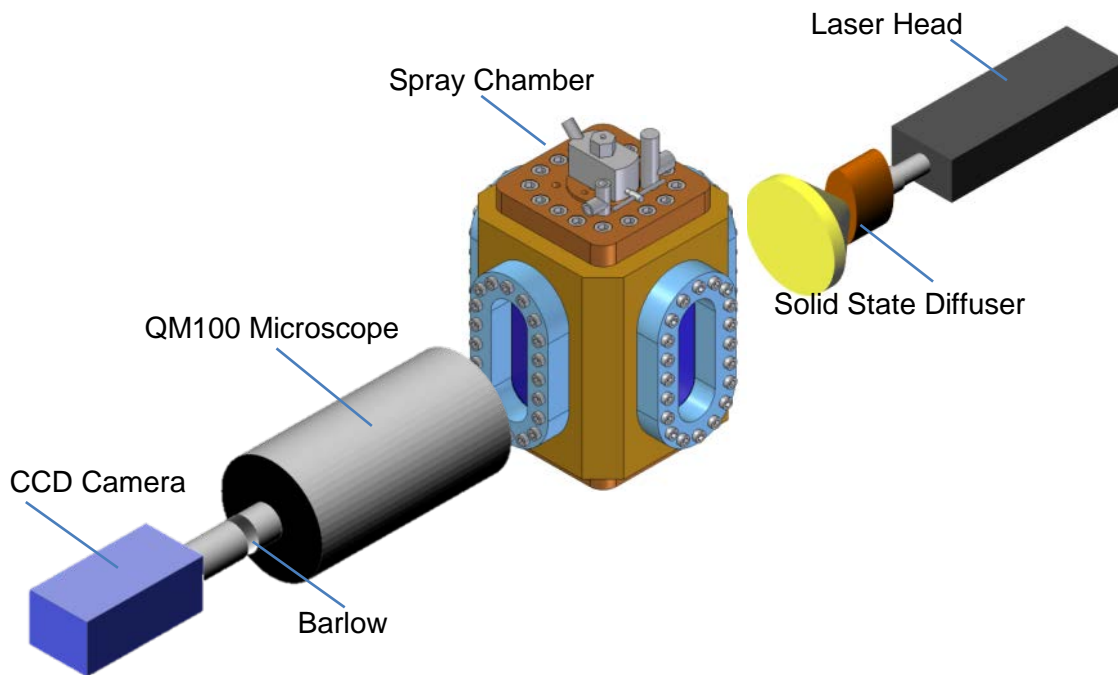
## 2. Methodology

### 2.1 Experimental apparatus

Non-evaporating diesel fuel spray measurements were conducted with a laser based imaging system in a constant volume High-Pressure Spray Chamber (HPSC). The HPSC operating volume is a square-section prism with rounded corners and the axis vertically oriented. Optical access to the injection test chamber is via three windows in the test chamber walls 80 mm thick, UV quality, optically polished

114 quartz, and viewing area of  $200 \times 70$  mm. The light source is a 120 milliJoule dual-cavity Nd:YAG laser  
115 capable of light pulses around 5 ns duration.

116 The chamber is pressurized to 30 bar with temperature and density of 298 K and  $35 \text{ kg/m}^3$ ,  
117 respectively, to give air density in the range of a heavy duty diesel engine. Diesel fuel is axially injected  
118 through a single solid cone fuel nozzle with an injection pressure of around 1200 bar from the top of the  
119 HPSC as shown in Figure 1.



120

121 **Figure 1.** Schematic view of the High-Pressure Spray Chamber showing laser and camera setup for  
122 shadowgraphy measurements.

123 The injection pressure profile which is highly repeatable from shot to shot is replicated based on the  
124 previous study of Bong et al [9]. The injector needle valve snaps open when the injector pressure achieves  
125 a given value, as determined by the tension of the needle valve spring. Needle lift is monitored using an  
126 eddy current proximity probe. It takes about 0.2 ms for the needle valve to lift completely.

The acquisition sequence is triggered by a pulse from the injector driver and the delay to the start of image acquisition is measured separately. The needle lift signal and the pulse generated by the laser were recorded using a digital oscilloscope to record the time at which the laser light pulse is activated, as indicated by the Q-switch pulse. Using shots obtained at the point where the spray is just starting to emerge from the nozzle, it is established that there is a delay of  $100 \pm 5 \mu\text{s}$  between start of injection and a significant response from the needle lift transducer. This information enables timing of subsequent shots.

A laser-based backlit imaging method (shadowgraphy) is used to investigate the micro-spray structure. As depicted in Figure 1, a Questar QM100 long distance microscope is attached to a LaVision Imager Intense dual-frame, 12 bit CCD camera with  $1376 \times 1040$  pixels. The camera and laser allow only two images to be taken for each shot of the injector. The delay between the two images can be as low as  $0.5 \mu\text{s}$ . The use of closely spaced images allows estimation of the propagation velocity of the leading edge of the injected fuel. An interval of about 30 s is allowed between injector shots to allow the chamber to settle.

The spray is backlit with laser light through a standard solid-state diffuser supplied by LaVision. The diffuser employs laser-induced fluorescent from an opaque plate impregnated with a fluorescent dye. The camera is focused, aligned, and calibrated on a graduated scale on the spray axis.

Two sets of microscopic data are achieved with and without using a Barlow lens. With the 2x Barlow lens, mounted between CCD Camera and Microscope, a magnification of 7.7:1, a field of view of  $1157 \times 860 \mu\text{m}$  and a spatial resolution of  $0.84 \mu\text{m}/\text{pixel}$  are achieved. These sets of data are used as a benchmark to validate the numerical results close to the nozzle exit.



## 148 2.2 Simulation setup

### 149 2.2.1 Mathematical method

150 In this study, the VOF phase-fraction based interface capturing technique similar to de Villiers et al  
 151 [11] is employed in the open source numerical code OpenFOAM v2.3. The code considers the two-phase  
 152 flow field as a single incompressible continuum with constant density  $\rho$  and viscosity  $\mu$ , including surface  
 153 tension. The compressibility effect will be included in future studies. The basic form of the governing  
 154 mass and momentum conservation are:

$$\nabla \cdot \mathbf{V} = 0 \quad (1)$$

$$\frac{\partial \rho \mathbf{V}}{\partial t} + \nabla \cdot (\rho \mathbf{V} \mathbf{V}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \int_{S(t)} \sigma \kappa' \mathbf{n}' \delta(\mathbf{x} - \mathbf{x}') dS \quad (2)$$

155 Where  $\mathbf{V}$  is the velocity,  $p$  is the pressure,  $t$  is the time,  $\boldsymbol{\tau}$  is the stress tensor,  $\kappa$  is the local curvature  
 156 of the liquid surface and,  $\mathbf{n}$  denotes a unit vector normal to the liquid surface  $S$ . The operators  $\nabla(\cdot)$  and  
 157  $\nabla \cdot (\cdot)$  represent the gradient and the divergence operations, respectively. The integral term in equation (2)  
 158 represents the momentum source due to surface tension force on the interface  $S(t)$ . This force only acts on  
 159  $S$ , as ensured by the indicator function  $\delta(\dots)$ . The time-varying phases interface  $S(t)$  is located  
 160 accordingly using a VOF surface-capturing approach which utilizes the volume fraction  $\gamma$  of diesel fuel as  
 161 an indicator function, defined as:

$$\gamma = \begin{cases} 1 & \text{for a point inside the liquid} \\ 0 < \gamma < 1 & \text{for a point in the transitional region} \\ 0 & \text{for a point inside the air} \end{cases} \quad (3)$$

162 The ‘transitional region’, where the interface is located, utilized as an artefact of the numerical  
 163 solution process. Fluid in a transition region is considered as a mixture of the two fluids on each side of  
 164 the interface, which cannot completely resolve a discontinuous step. The transport equation for the  
 165 indicator function is:

$$\frac{\partial \gamma}{\partial t} + \nabla \cdot (V\gamma) = 0 \quad (4)$$

According to the definitions of  $\gamma$ , the local thermo-physical properties are given by:

$$\rho = \gamma \rho_l + (1 - \gamma) \rho_g \quad (5)$$

$$\mu = \gamma \mu_l + (1 - \gamma) \mu_g \quad (6)$$

where the subscripts  $l$  and  $g$  represents the liquid and gas, phases respectively.

The LES/VOF equations are derived from equations (1), (2) and (4) using localized volume averaging of the phase-weighted hydrodynamics variables. This process known as filtering, includes decomposition of the relevant variables into resolvable and sub-grid scales of turbulent fluctuations. As the results of the filtering process, the sub-grid scale fluctuations will be eliminated from direct simulation. This filtering together with the non-linear convection terms in equation (2) introduce an additional quantity, comprising correlation of the variable fluctuations at sub-grid scales that entail closure through mathematical models, known as the subgrid scale (SGS) stresses  $\tau^{sgs}$  as they signify the influence of the unresolved small scales of turbulence, given by:

$$\tau^{sgs} = \overline{V\overline{V}} - \overline{V}\overline{V} \quad (7)$$

and estimated by a single subgrid scale model of the eddy-viscosity type:

$$\tau^{sgs} - \frac{2}{3} k \mathbf{I} = - \frac{\mu^{sgs}}{\rho} (\nabla \overline{V} + \nabla \overline{V}^T) \quad (8)$$

where  $k$  is the subgrid scale turbulent energy and  $\mu^{sgs}$  is the subgrid scale viscosity, both are determined from the one-equation SGS turbulent energy transport model accredited to Yoshizawa [37].

$$\frac{\partial k}{\partial t} + \nabla \cdot (k\overline{V}) = \nabla \cdot [(v + v^{sgs})\nabla k + \tau^{sgs} \cdot \overline{V}] - \varepsilon - \frac{1}{2} \tau^{sgs} : (\nabla \overline{V} + \nabla \overline{V}^T) \quad (9)$$

179 where  $\varepsilon = C_\varepsilon k^{2/3}/\Delta$  is the SGS turbulent dissipation rate,  $\nu^{sgs} = C_k k^{1/2}/\Delta$  and  $\Delta = \sqrt[3]{V}$  is the SGS  
180 length scale where  $V$  is volume of the computational cell. The coefficients, found from statistical  
181 considerations, are  $C_k = 0.05$  and  $C_\varepsilon = 1$  [6].

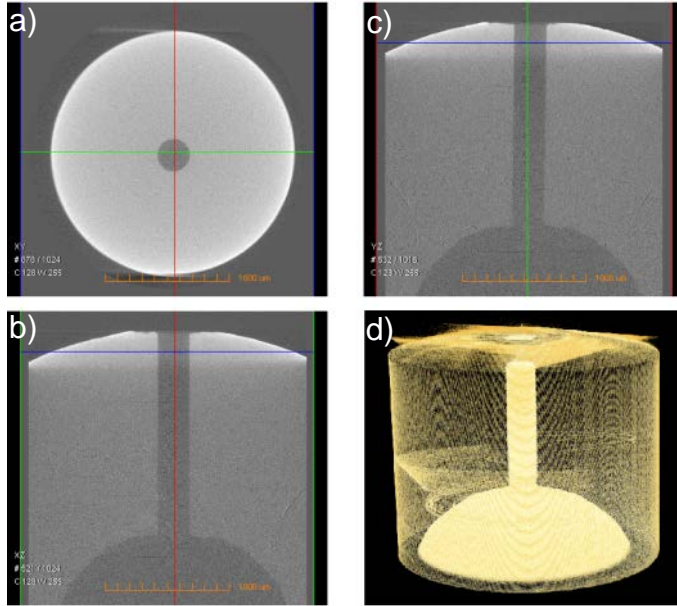
### 182 2.2.2 The Numerical solution method

183 Mathematical models for this simulation are solved using an implicit finite-volume method, which  
184 employs spatial and temporal discretization schemes. This method preserves a sharp interface resolution  
185 by including a compression velocity term [38] in the phase transport equation, acting to compress the  
186 VOF interface. The solution procedure utilizes the Pressure Implicit with Split Operator (PISO) algorithm  
187 [39], together with conjugate gradient methods for coupled solution of mass and momentum conservation  
188 equations which is specifically suited to transient flows [40].

189 In order to preserve the proper physical limits on the fluid-dynamics variables, different integration  
190 schemes are tried from highly dissipative up to highly conservative. In this study, the advection terms are  
191 solved by the Normalized Variable (NV) Gamma differencing scheme [41]. A conservative, bounded,  
192 second-order scheme is used for Laplacian derivative terms and a second-order, implicit discretization  
193 scheme is used for time derivative terms. The numerical integration time-step is adjusted by various  
194 stability criteria, and is of the order  $1 \times 10^{-9}$  s for the fine case.

### 195 2.2.3 Boundary conditions and initial setup

196 Atomization is affected by the design of the sac and nozzle orifice inlet which consequently influence  
197 primary breakup [8, 14, 18]. The computational domain has therefore been modelled using the geometry  
198 of the experimental nozzle determined using X-ray Computer Aided Tomography (CAT) analysis as  
199 shown in Figure 2. This analysis reconstructs the images with pixel numbers of  $1016 \times 1024 \times 1024$ , and  
200 effective voxel size of  $2.318 \mu\text{m}$ .



**Figure 2.** X-Ray Tomography measurement of sac and nozzle geometry and dimensions. a) X-Y view; b) X-Z view; c) Y-Z view and d) 3D view of nozzle. Images provided by The Centre for Materials and Surface Science and the Centre of Excellence for Coherent X-ray Science at La Trobe University, employing an Xradia MicroXCT instrument.

All the experimental conditions were replicated in numerical models including the sac volume inlet, spray chamber pressure and air and diesel fuel temperature and viscosity. Fuel properties and set up conditions are listed in Table 1. The sac inlet pressure is ramped from 30 bar initially to 850 bar after 50  $\mu\text{s}$  then to 1200 bar after a further 25  $\mu\text{s}$  then constant at 1200 bar to the end of simulation. This is to some extent arbitrary but is premised on published data implying that the sac pressure rises rapidly during needle opening [1, 42-44]. For instance, Moon et al. [1] found that quasi-steady stage jet velocity was reached when the needle lift was only 17% of the maximum needle lift. The ramp was chosen to give an approximate match of modelled and experimental penetration rates. The lower pressure rise rate in the second 25  $\mu\text{s}$  was adopted to avoid numerical instabilities.

In the present study, it was found that the duration of the needle lift is about 200  $\mu\text{s}$  and that the signal from the eddy current needle lift transducer signal has a delay of around  $100 \pm 5 \mu\text{s}$  compared to actual needle lift. This is determined by observing the timing of the laser Q-switch signal relative to the

218 needle lift signal for shots where the captured image shows the spray just starting to emerge from the  
 219 nozzle. Thus, the needle lift signal could not be used to determine instantaneous needle position. The  
 220 maximum needle lift is about 200  $\mu\text{m}$ .

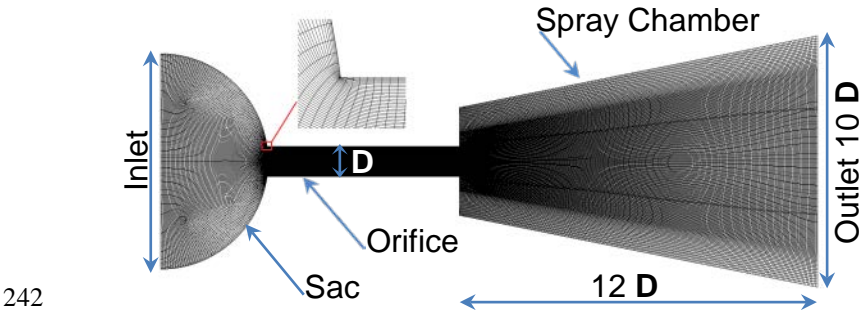
221 **Table 1.** Fuel properties and operating conditions based on experimental setup [45]. \* Injection velocity,  
 222 Weber and Mach numbers are for the quasi-steady stage of spray [45]. The nozzle diameter is used as the  
 223 length scale.

Parameter	Value
Injection pressure	120 MPa average
Nozzle diameter	0.25 mm
Nozzle length	1.6 mm
Nozzle nominal geometry	$K_s = 0$
Fuel	Diesel
Diesel fuel density	832 $\text{kg/m}^3$
Gas	Compressed air
Density ratio	42
Fuel Kinematic viscosity	$2.52 \times 10^{-6} \text{ m}^2/\text{s}$
Surface tension	0.03 N/m
Temperature	25°C
Fuel $Re_l$	$7000 \leq Re \leq 37000$
*Indicative injection velocity	367
*Fuel Mach number	$367 / 1250 = 0.3$
* $We_l$	933843
*Ohnesorge number	0.077
Chamber pressure	30 bar

224 The nozzle orifice at the start of each injection in the experimental injections is not necessarily full of  
 225 fuel due to needle bounce and dribble phenomena at closure nor empty of fuel due to cohesive and  
 226 adhesive forces. Hence for a good comparison of modelled and measured injection, a method for  
 227 determining the position of the liquid-gas interface in the nozzle orifice at the start of injection was  
 228 implemented. Firstly, the sac and three quarters of the nozzle were filled with diesel fuel at a pressure of  
 229 30 bar and then the sac inlet pressure raised as described above. Later on, at the end of the injection cycle  
 230 when the needle closes, the boundary condition is changed from inlet to wall to prevent any further fuel  
 231 entering the sac, emulating the needle valve closure process. The result of this simulation is that the

nozzle fills with liquid to 5.2 D (81% of the nozzle length) from the nozzle entrance. This is due to the equilibrium between adhesive forces, surface tension of the liquid phase and hydrodynamic forces amongst liquid and pressurized air in the spray chamber. The position of the liquid-gas interface inside the nozzle orifice resulting from this simulation (at 5.2 D) is used to initialize the main simulation. This starting point is somewhat arbitrary but goes some way to accounting for air ingestion as described in [42-44, 46].

Considering the boundary layer, atomization zone and no-slip condition at the walls (sac and orifice), a hexahedral structured mesh was generated as shown in Figure 3. It has been reported that the spray structure is not axisymmetric [5, 9, 14, 34, 45], therefore the full computational domain ( $360^\circ$ ) of the atomization zone is meshed.



**Figure 3.** Computational domain and boundary conditions (coarse case, with refined mesh in the orifice and atomization regions).

In order to conduct a mesh sensitivity study, three different mesh resolutions are generated with coarse (4 million cells), medium (8 million cells), and fine grids (20 million cells). Cell size is refined down to  $0.1\ \mu\text{m}$  in the orifice and  $1.7\ \mu\text{m}$  in the primary atomization zone in the finest resolution case. This cell size can capture droplets down to the  $10\ \mu\text{m}$  range based the optimistic premise that 5 cells can give reasonable representation of a single droplet [20]. The resolution of these cases, time-step range, number of CPUs, and computational cost (wall clock time) for each case are summarized in Table 2.

**Table 2.** Summary of mesh parameters for numerical models

Case	Average Resolution ( $\mu\text{m}$ )			Cell count	Time Step ( $\times 10^{-9}$ S)	CPU (core count)	Wall clock time (hours)
	Sac	Orifice	Spray Chamber				
Coarse	13	2	6.5	$4 \times 10^6$	$1.6 \leq \Delta T \leq 80$	128	151.4
Medium	7.5	1.2	5	$8 \times 10^6$	$1.2 \leq \Delta T \leq 60$	256	225.8
Fine	4	0.5	3.5	$20 \times 10^6$	$0.9 \leq \Delta T \leq 30$	384	565.3

Being aware of the importance of in-nozzle generated turbulence on primary atomization [18, 20], in the fine case, special consideration was given to generating the mesh inside the nozzle orifice. The size of cells in the orifice were decreased to the order of the Kolmogorov length scale for the liquid phase,  $\eta_l$ , to assure that the smallest generated eddies, as a result of boundary layer and change in cross sectional area, are well resolved. The smallest length scales associated with the flow field for the quasi-steady stage of spray are reported in Table 3. It can be seen in this table that  $\eta_l$  is much larger than mesh size in the nozzle for the finest grid. To resolve a given length scale it is necessary that  $\eta_l \geq 2\Delta x$ , where  $\Delta x$  is the grid size [41]. This mesh resolution leads to the proper prediction of small eddies of the liquid phase inside the nozzle orifice in the fine resolution case. A sub-grid scale model is needed for the turbulence in the gas phase.

**Table 3.** Kolmogorov length scales for the liquid and gas phases of the quasi-steady stage of spray where the turbulence intensities used are 4.4 % and 10 %, respectively.

Parameter	Value
Liquid phase Kolmogorov length scale, $\eta_{\text{liq}}$	$0.7 \mu\text{m}$
Minimum mesh size in nozzle hole for fine case, $\Delta x_{\text{min}}$	$0.1 \mu\text{m}$
Gas phase Kolmogorov length scale, $\eta_{\text{gas}}$	$0.008 \mu\text{m}$
Minimum mesh size in spray chamber for fine case, $\Delta x_{\text{min}}$	$1.7 \mu\text{m}$

#### 2.2.4 Mesh sensitivities

In this research structured grids are used to achieve higher quality and control which may be sacrificed in unstructured and hybrid meshes. In addition, the efficiency of the differencing scheme for

265 bounding the convection term of the transport equations in a structured mesh is much higher in  
266 comparison to an unstructured mesh [47].

267 It is possible that the present conically stretched grid leads to greater spray angle than a purely  
268 Cartesian/orthogonal grid, for example. The core of the mesh is purely Cartesian/orthogonal, and the  
269 divergence immediately adjacent to the core region is less than near the outer boundaries. Using a  
270 structured mesh as in the present study reduces the effects of divergence from orthogonality. A non-  
271 orthogonality corrector is employed in the numerical solution to minimize any possible grid orientation  
272 influences.

### 273 3. Results and discussions

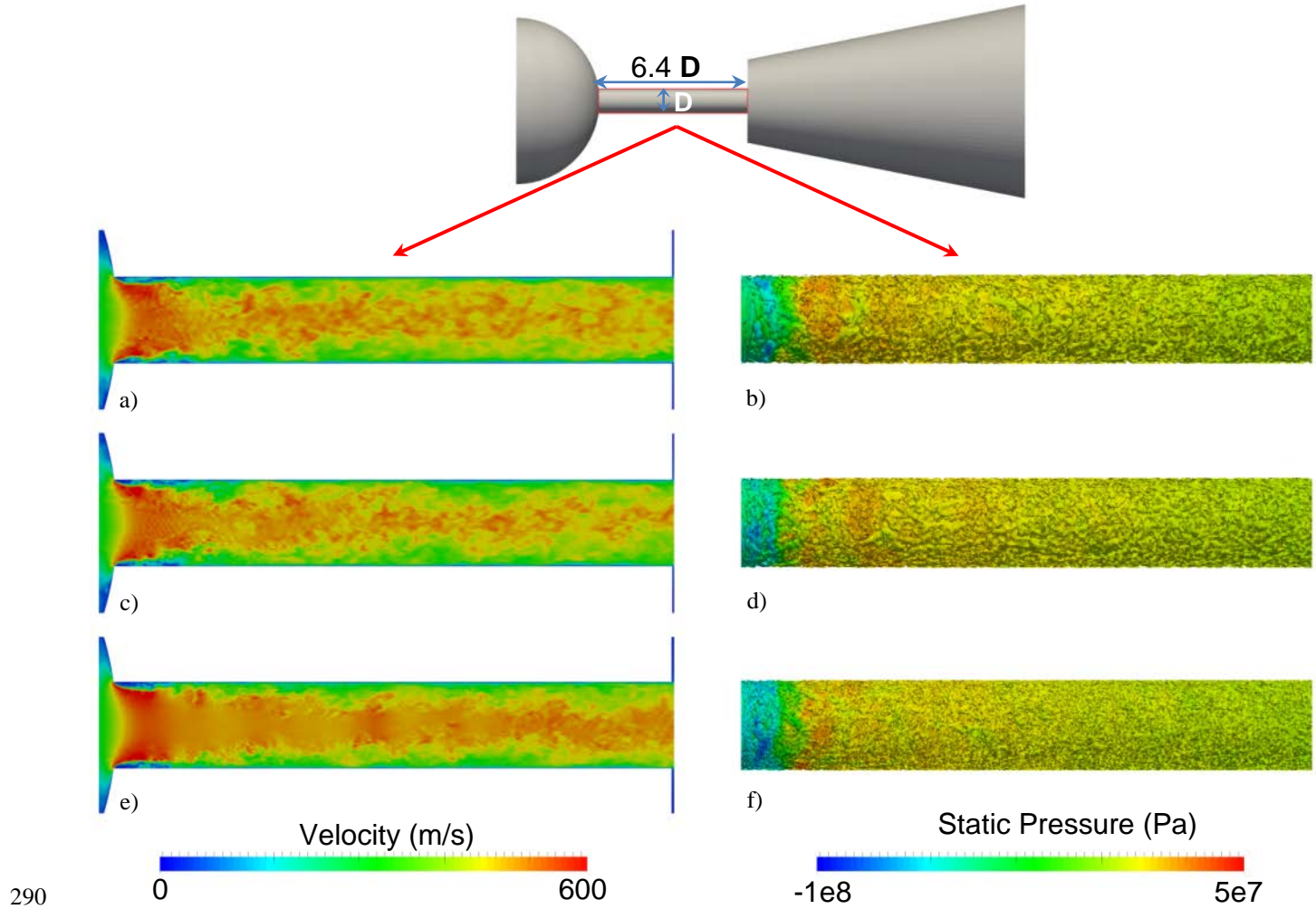
274 Due to the unavailability of a transparent orifice, only images of the spray in the chamber are  
275 presented. The comparisons between simulations and experiments are qualitative and focus on the overall  
276 spray shape, surface irregularities, spray penetration and generated droplets. The numerical data presented  
277 in the next two sections are obtained by means of the second-order time derivatives method and the NV  
278 Gamma scheme for solving the convection terms.

#### 279 3.1 In-nozzle turbulence

280 Figure 4 illustrates the influence of mesh resolution on turbulent eddies, generated and developed  
281 within the orifice boundary layer leading to small/large-scale irregularities. These irregularities are the  
282 origin of jet surface instabilities. This Figure shows a zoomed view of the jet turbulent structures inside  
283 the nozzle orifice demonstrating the small-scale eddies in each case at the quasi-steady stage (sac inlet  
284 pressure of 1200 bar and Re of 37000 at the orifice exit). In the left column (images *a*, *c*, and *e*), in-nozzle  
285 flow is coloured by velocity magnitude. In the right column at corresponding times (images *b*, *d*, and *f*),  
286 the turbulent eddies are depicted using a Q-criterion isosurface of  $5 \times 10^9$ , coloured by static pressure.  
287 Negative static pressures after the nozzle entrance are due to the absence of a cavitation model. In the



high-resolution case, smaller eddies have been resolved demonstrating the importance of mesh resolution on predicting upstream flow conditions.



**Figure 4.** Jet liquid turbulent structures at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar and  $Re = 37000$  at the orifice exit for coarse (a and b), medium (c and d) and fine (e and f) mesh cases. In the left column (images a, c, and e), in-nozzle flow is coloured by velocity magnitude. In the right column at corresponding times (images b, d, and f), the turbulent eddies are illustrated using a Q-criterion isosurface of  $5 \times 10^9$ , coloured by static pressure. Negative static pressures after the nozzle entrance are due to the absence of a cavitation model. Greater resolution of jet core and boundary layer turbulence are apparent with increasing mesh density.

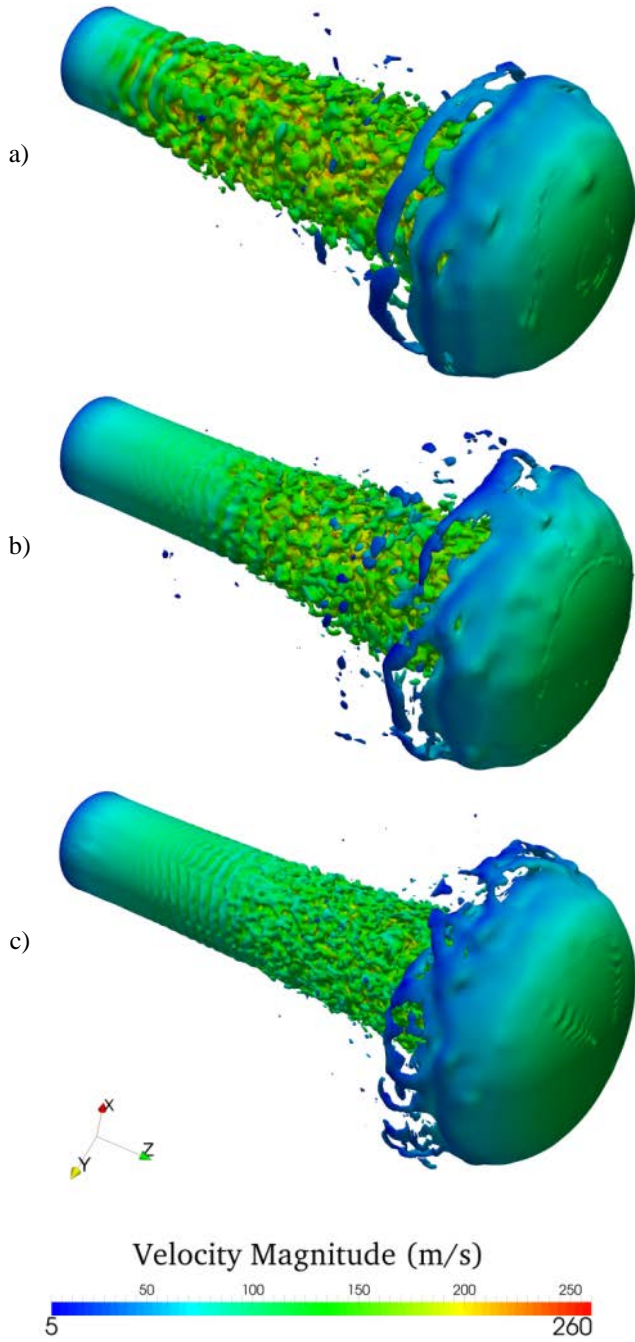
### 3.2 Morphology of the penetrating jet

Some instantaneous features such as flow structures and the evolution of spray transients are presented in Figure 5 for three different mesh resolutions at  $15 \mu s$  after start of penetration (ASOP)

301 showing the influence of mesh size on capturing surface instabilities. The umbrella-shaped leading edge  
302 of the jet for coarse, medium, and fine cases shows a smooth surface with penetration velocity of 123 m/s  
303 in agreement with DNS results [14, 34] for similar velocity ranges.

304 The irregularities on the trailing edge of the umbrella play a significant role in the disintegration  
305 process of the penetrating jet. As can be seen in Figure 5, finer grids lead to capturing more waves  
306 resulting in higher fragmentation rates.

307 Mesh resolution affects prediction of instabilities on the liquid jet behind the umbrella. In-nozzle-  
308 generated turbulence in combination with relaxation of the velocity profile at the nozzle exit initiate the  
309 perturbations leading to wave growth on the jet surface. As can be seen in Figure 5, surface instabilities  
310 are triggered close to the nozzle orifice exit (further than one diameter for the fine grid) as a result of the  
311 K-H mechanism (wave generation on jet surface based on aerodynamic interaction, creating ligaments  
312 which then either disintegrate to produce droplets or just roll up and continue to develop).

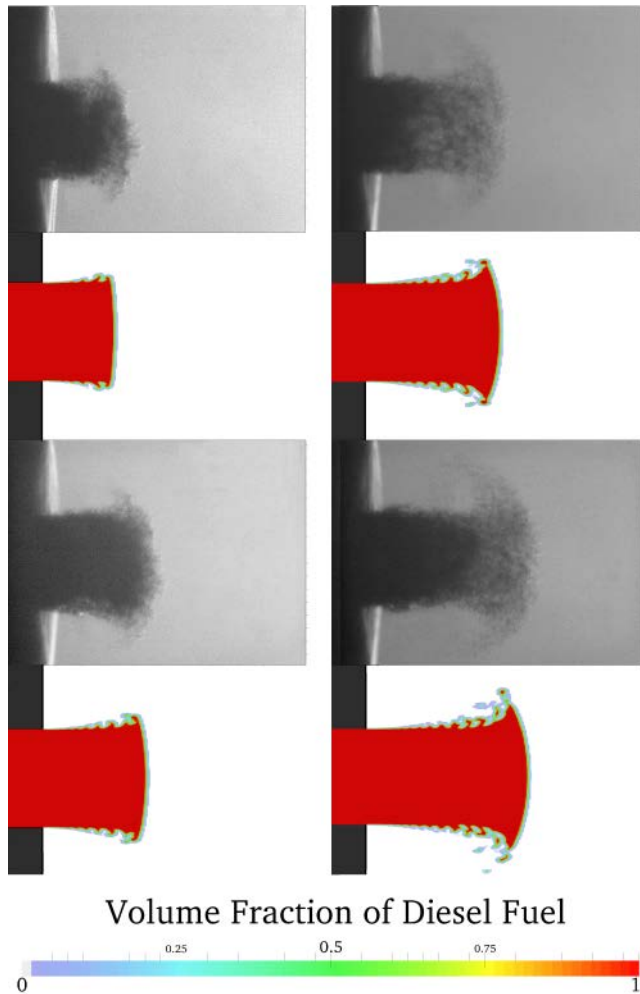


**Figure 5.** Structure of the jet colored by velocity magnitude at 15  $\mu\text{s}$  ASOP, indicated by liquid interface of  $\gamma = 0.5$ , for coarse (a), medium (b) and fine (c) mesh cases showing over-prediction of breakup for the coarse case and the resolution of smaller scale surface instabilities and breakup for the finer case.

Inaccurate prediction of the velocity relaxation at the liquid-gas interface due to insufficient grid resolution intensifies the K-H mechanism, exaggerating the liquid jet disintegration process. Furthermore, the thickness of ligaments is a matter of the cell size where the pinching-off occurs as the thickness drops

below the cell size, followed by the generation of several droplets of varying sizes [8, 48, 49]. It can be concluded that the mesh density at the air-fuel interface considerably influences the development of ligaments and the breakup process.

Figure 6 shows a comparison of experimental images with the numerical results with the fine mesh case at different times ASOP. Adding a 2× Barlow lens to the microscope to give a total magnification of 7.7:1 enables greater details of the early spray to be captured. The use of a dual frame CCD camera with a time interval of one microsecond between subsequent images allows validation of the velocity of advance of the leading edge and tracking of the transient changes in the morphology of the penetrating diesel jet.



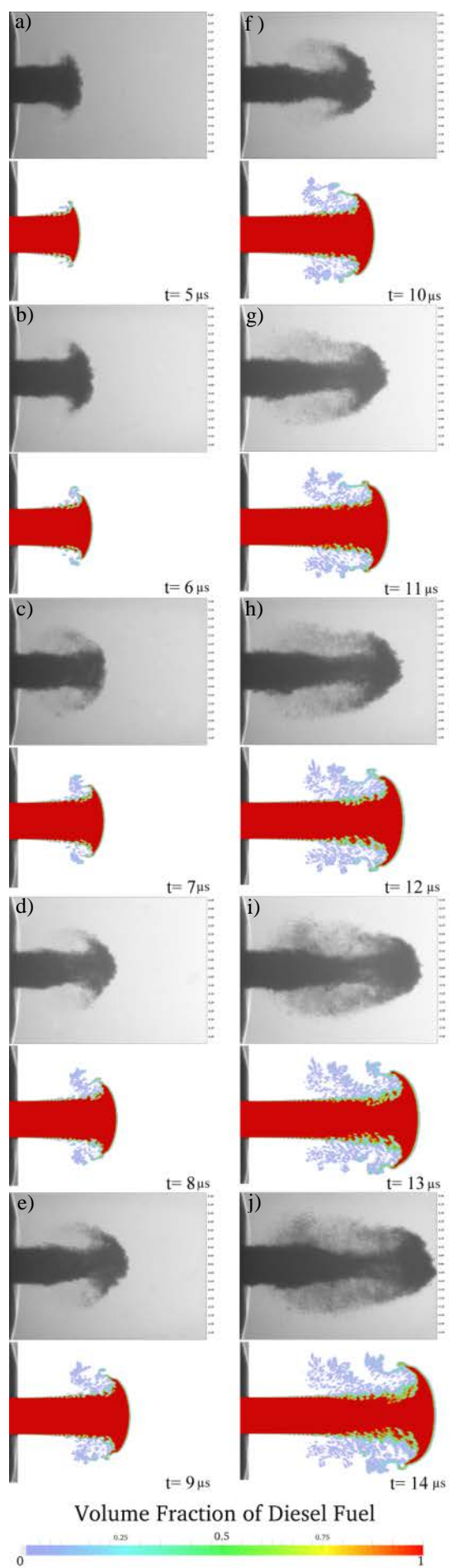
**Figure 6.** Comparison of experimental images with numerical results for the fine mesh case with highest magnification. Each experimental image is from a different injection event, apart from the first two (a and b) which are captured from two consecutive frames with 1  $\mu$ s inter frame time.

Some transparency can be clearly seen in the shadowgraphy images. This is due to air inclusion within the liquid inside the orifice, left from previous injection. The existence of ingested air inside the injector was reported by Swantek et al. [46] at the end of injection (EOI) process. Air inclusion inside the injector influences the spray structure and could be a source of observed deviation between experimental and numerical results.

Shadowgraphy images are compared with the numerical results in Figure 7 with a larger field of view, presenting the general structure of the diesel spray. In this Figure, images *a* and *b*, *d* and *e*, *g* and *h*, *i* and *j* are paired, each pair is captured from the same injection event with one microsecond delay between consecutive frames.

The experimental images illustrate a more structured surface even very close to the nozzle exit compared with the numerical results. The leading edge of the emerging jet is disintegrating unlike the numerical results where the leading edge umbrella-shaped structure of the emerging jet is continuous liquid with breakup occurring more rapidly around the periphery. Air inclusion prior to start of injection could explain the rougher surface, and earlier disintegration of the leading edge in the experimental images resulting in the more oblique angle of the umbrella.

The necking of the jet length behind the umbrella can be obviously seen in the experimental images in Figure 7, while it is not as marked in the simulations. The difference is possibly related to the presence of air in the experimental jet, as indicated by partial transparency of the experimental images, and thus more rapid disintegration. The outer recirculating gas flow removes the generated droplets and advects them toward the outer flow which can be seen in images *i* and *j* of Figure 7.

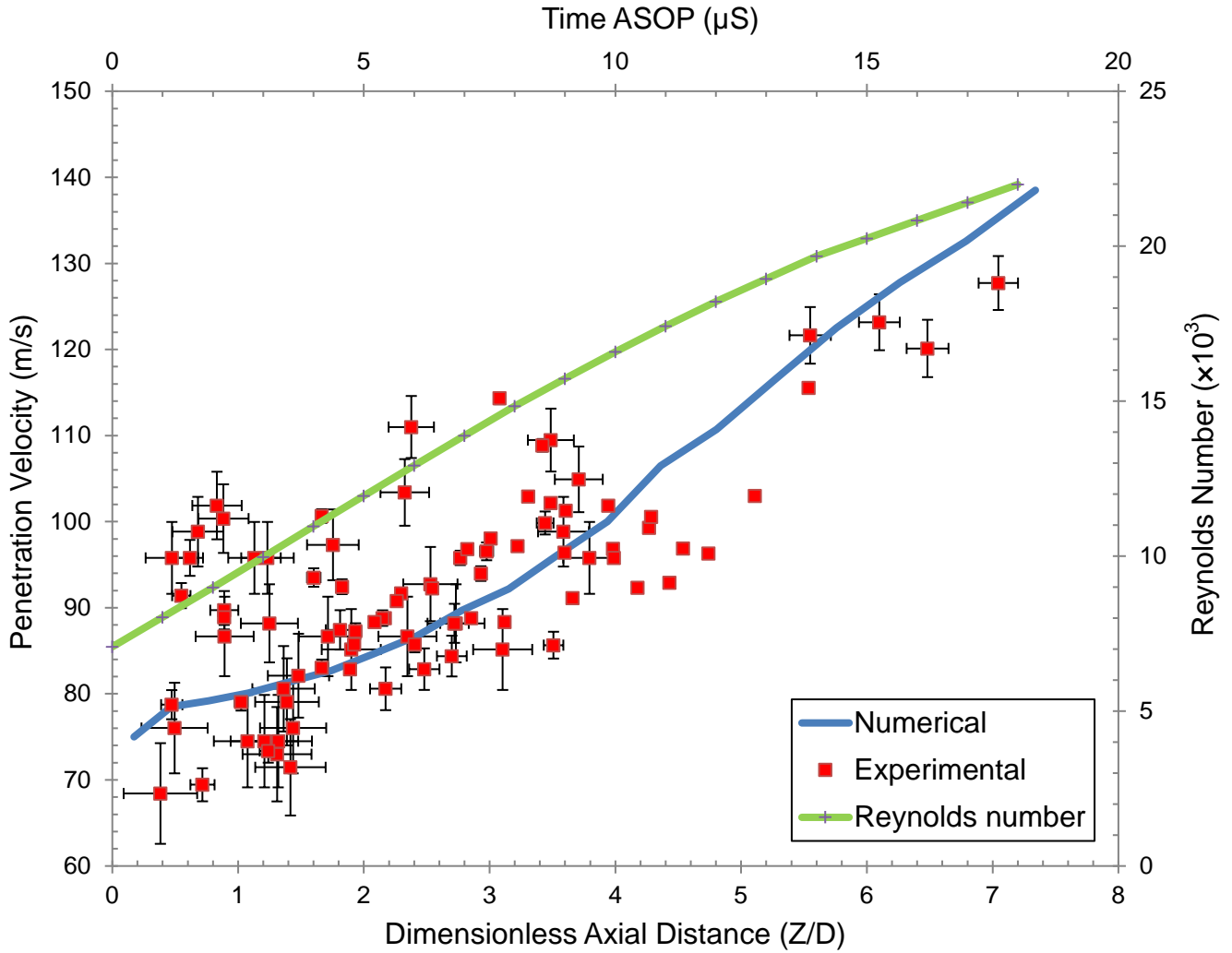


353 **Figure 7.** Comparison of experimental (with no magnification) and numerical results. Numerical results  
354 shown are for the fine mesh, colored by volume fraction of diesel fuel. Images a and b, d and e, g and h, i  
355 and j are paired, captured from the same injection event from two consecutive frames with  $1\ \mu\text{s}$  inter  
356 frame time.

357 Further differences between the experimental and numerical results are in the production of small  
358 droplets in the experimental images but not in the numerical results. This is due to the constraint in  
359 computational resources where the grid resolution in the computational domain is insufficient to resolve  
360 the small eddies in the air phase which influences the breakup processes of the ligaments and droplets.

361 Capturing two subsequent images enables velocity measurement of the jet leading edge.  
362 Experimental values for 100 double frame shots, with inter-frame times varying between 1 to  $15\ \mu\text{s}$  are  
363 shown in Figure 8. The error bars are based on the accuracy of the detection of the leading edge of the jet  
364 and this is a function of the inter-frame time. The jet penetration velocity at various axial distances from  
365 nozzle exit with corresponding time ASOP, demonstrated in Figure 8, show good agreement between  
366 numerical and experimental results. The  $Re$  is based on the average axial velocity at the nozzle exit.

367 Instantaneous mass flow rate was not measured. Quasi-steady mass flow rate was measured at  
368  $0.0139\ \text{kg/s}$  and numerically predicted at  $0.0168\ \text{kg/s}$ . The difference is assumed to be due primarily to  
369 the absence of cavitation in the simulations.



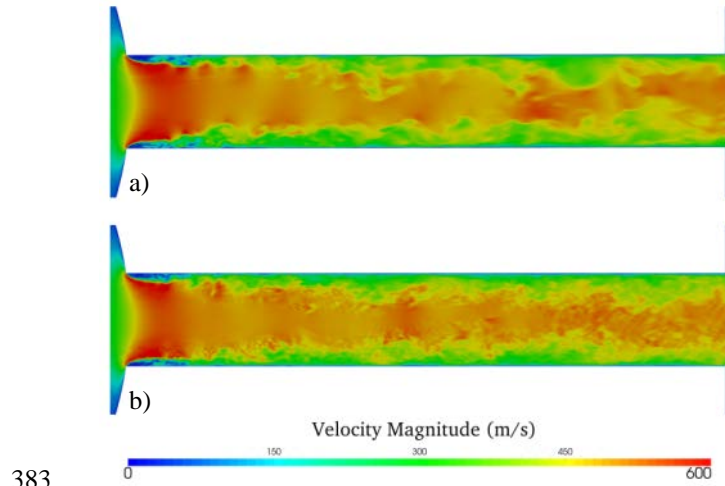
**Figure 8.** Comparison of measured and predicted jet penetration velocity at various axial distances from nozzle exit with corresponding times ASOP. Re values, from computation, are calculated using the average velocity of liquid at the nozzle exit.

### 3.3 Numerical schemes

The behavior of different interpolation schemes is presented in Figure 9, Figure 10, and Figure 11. The order of the temporal integration schemes for phase-fraction and governing conservation equations plays a significant role in prediction of small-scale eddies inside the nozzle orifice. As depicted in Figure 9, at the quasi-steady stage, employing the second-order scheme named *Backward* results in smaller scale eddies in comparison to the first-order, *Euler*, approach due to higher dissipation in the first-order scheme. This influences irregularities which are mainly generated by the reduction of the cross-sectional

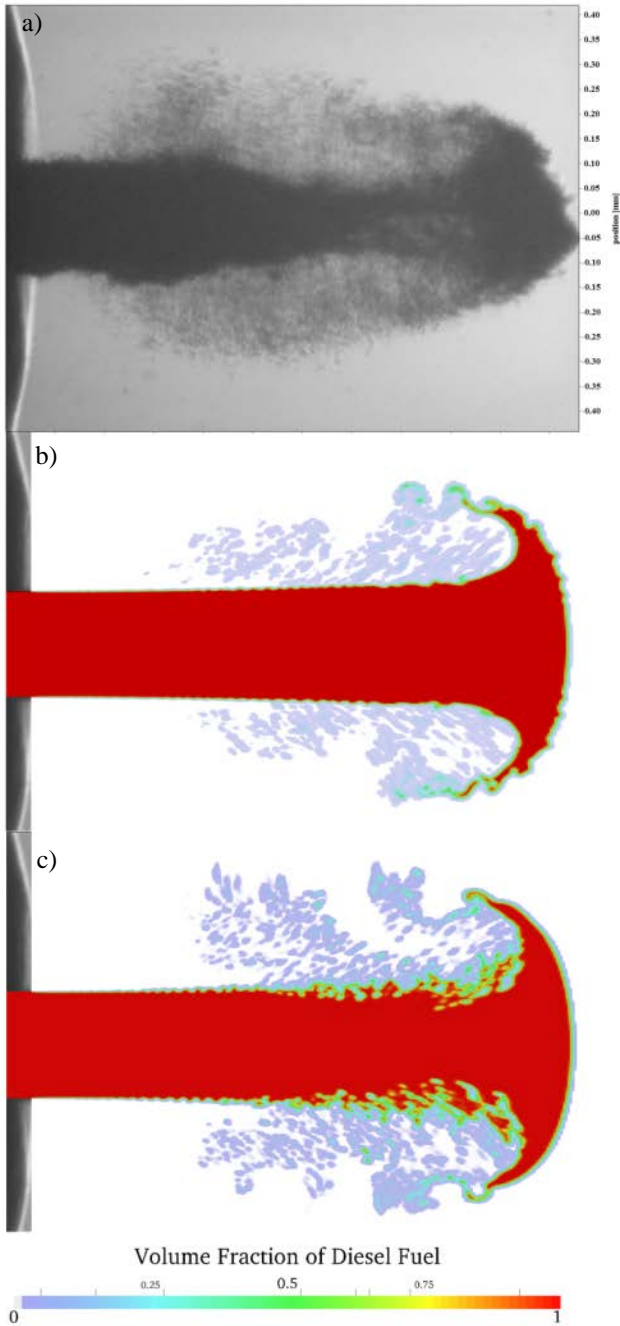


area at the nozzle inlet where there is strong change in flow direction, and vena contracta phenomena [50].



**Figure 9.** Influence of the time derivative order on prediction of turbulent structures within the nozzle orifice at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar), colored by velocity magnitude, for the fine grid case with; a) Euler, first-order and b) Backward, second-order.

The first-order discrete equations are more diffusive than the second-order discrete equations [41]. The impact of the time interpolation method is also seen in Figure 10, at  $14 \mu\text{s}$  ASOP. The disintegration of droplets from the liquid jet surface behind the leading edge diminishes with the first-order scheme compared with the second-order scheme. The second-order accurate interpolation scheme enables modelling of smaller fluctuations of velocity in the liquid-gas interface. Therefore, the K-H waves intensify behind the umbrella-shaped leading edge resulting in higher rates of separation. This separation narrows the liquid jet, demonstrating the necking phenomena of the spray. This necking process is weakened in the first-order interpolation scheme due to higher dissipation (in-efficiency in resolving smaller eddies) in this method. This is why the second-order scheme for time derivatives has been employed for the present study.

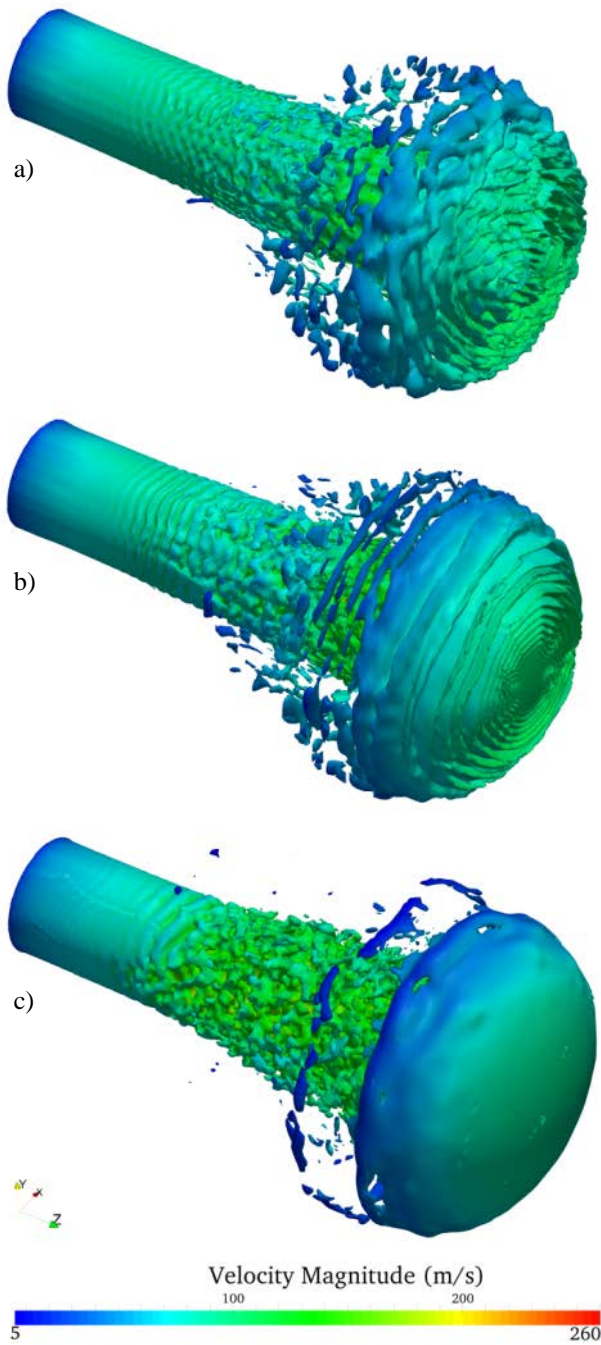


**Figure 10.** Comparison of an experimental image with numerical results showing the effect of the order of temporal integration scheme on the jet disintegration process at  $t = 14 \mu\text{s}$  ASOP, colored by volume fraction of diesel fuel, for the fine resolution case; a) Experiment, b) First-order, and c) Second-order.

The influence of the convection-specific interpolation scheme on capturing the liquid-gas interface is illustrated qualitatively in **Figure 11** for medium grid resolution. Different ranges of first/second order bounded numerical schemes have been investigated from the more dissipative, Total Variation Diminishing (TVD), up to the more conservative NV schemes. The NV Gamma scheme showed a

smooth leading edge surface which is in agreement with DNS results of [14, 34] at a similar penetration velocity. Thus, the NV Gamma scheme has been selected for solving the convection terms. The presence of air in the liquid could play a role in the generation of surface roughness in the leading edge of the experimental jet which is not seen in the simulations.

Secondary interfacial instabilities known as Rayleigh-Taylor (R-T) instabilities may develop when the propagation velocity is sufficient to exceed a critical value. If R-T instability develops, it presents as a rapid crosswise modulation on the leading edge followed by shedding of drops [11]. These interfacial instabilities grow as the jet proceeds downstream and increase gas penetration into the core liquid. The latter forms ‘blobs’ joined by thin core ligaments. These blobs finally snap and complete the core breakup process. The simulations capture an umbrella-shaped leading edge which qualitatively is in agreement with the experimental results as shown in Figure 6 and Figure 7, although no spanwise instabilities due to the R-T mechanism are apparent with the NV Gamma scheme. Figure 11 demonstrates that certain convection interpolation schemes may give apparent or Rayleigh-Taylor (R-T)-like instabilities which are not necessarily physical.

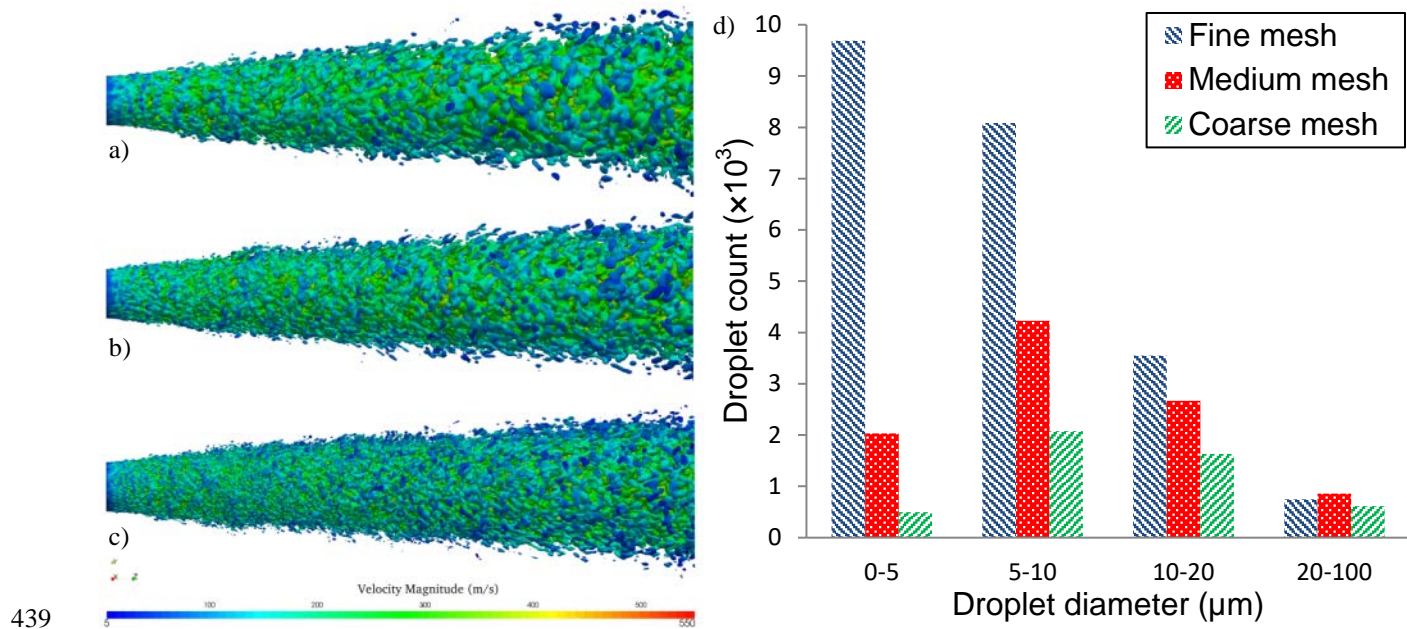


**Figure 11.** The effect of convection-specific interpolation schemes on capturing surface instabilities of the jet beyond the nozzle exit for the medium resolution grid at  $t = 14 \mu\text{s}$  ASOP, indicated by volume fraction of  $\gamma = 0.5$ , and colored by velocity magnitude; a) TVD, FilteredLinear, b) TVD, LimitedLinear, and c) NV, Gamma

### 3.4 Spray structure of diesel fuel at quasi-steady operating condition (pressure = 1200 bar)

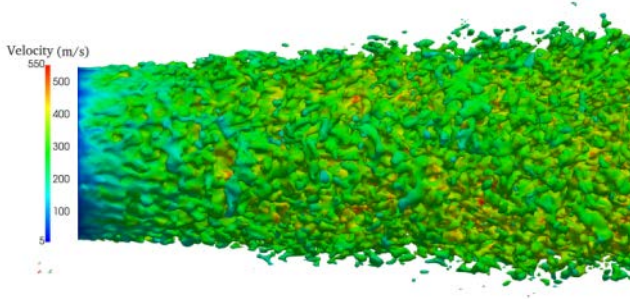
The atomized liquid fraction on the spray surface for the three mesh resolutions is illustrated in Figure 12 by  $\gamma = 0.1$  isosurfaces, coloured by the velocity magnitude at the quasi-steady stage where

427 diesel fuel pressure at sac inlet is 1200 bar. The onset of primary atomization can be seen close to the  
 428 nozzle exit for the three mesh resolutions. Very fine droplets are captured near the nozzle exit noticeably  
 429 in the finest case (20 million cells) which agrees with the experimental images. The surface velocity  
 430 decelerates rapidly close to the orifice exit due to relaxation of the velocity profile. The number of  
 431 discrete droplets captured for the coarse, medium and fine meshes at the quasi-steady stage are 4830,  
 432 9494, and 22076 respectively. The increase in apparent atomization from finer meshes is due to better  
 433 prediction of the smaller-scale in-nozzle turbulent structures as presented in Figure 4, resulting in smaller-  
 434 scale surface eddies which intensify the breakup process. Consequently, the breakup rate increases in  
 435 cases with higher mesh resolution. The atomization rate at the quasi steady stage is 0.0139, 0.0148, and  
 436 0.0158 kg/s for coarse, medium and fine mesh, respectively. The finer the mesh, the finer the resolved  
 437 droplets. Mesh independence is not demonstrated due to limited computer resources and unfeasible  
 438 computation time.



440 **Figure 12.** Spray morphology within 12 nozzle diameters of the nozzle exit, indicated by isosurface of  
 441 volume fraction  $\gamma = 0.1$ , colored by velocity magnitude at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar); a) Coarse,  
 442 b) Medium and c) Fine case showing decreasing scale of surface features with increasing mesh resolution.  
 443 Panel d) shows quantitatively the greater number of fine droplets generated with finer meshes.

444 Figure 13 illustrates a close-up view of the jet disintegration, visualized using the isosurface of  
 445  $\gamma = 0.5$  for the fine mesh case, at the quasi-steady stage. This picture represents the jet surface detachment  
 446 and droplet generation, occurring even at one nozzle diameter downstream.

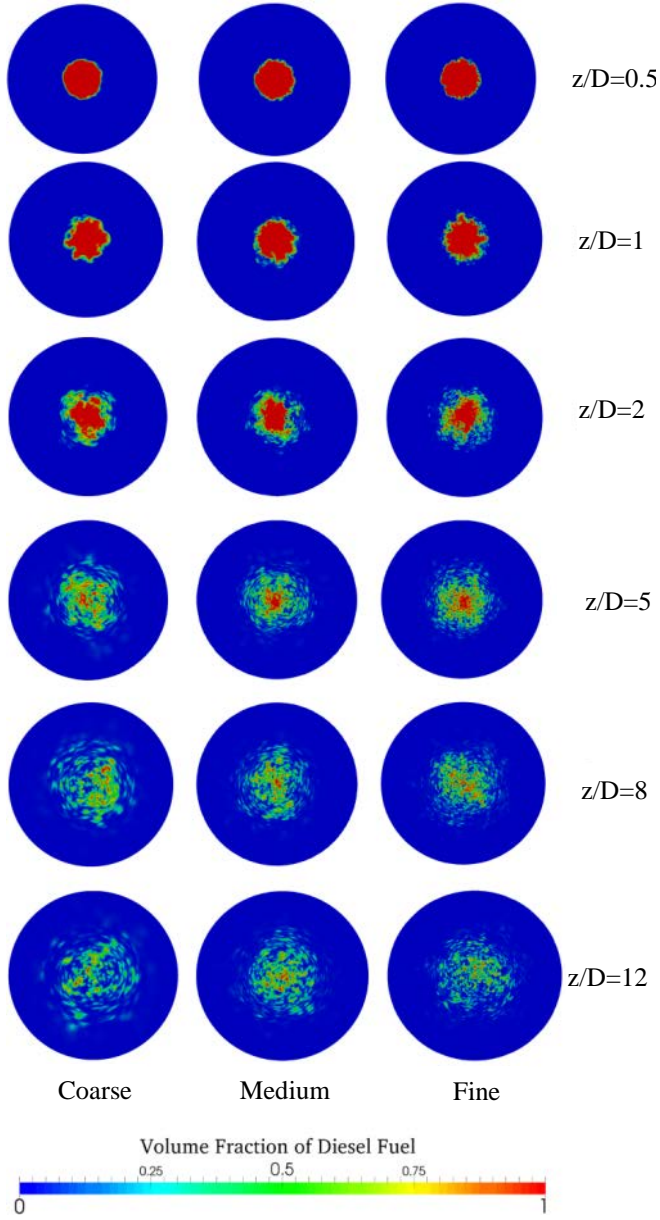


447

448 **Figure 13.** Close-up view showing the onset of surface breakup visualized by isosurface of  $\gamma = 0.5$   
 449 colored by velocity for the fine mesh case at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar).

450 The growth of non-axisymmetric disintegration at different cross-sections from the nozzle exit is  
 451 presented in Figure 14. The formation of small longitudinal waves can be seen at one nozzle diameter  
 452 downstream of the nozzle exit. At one diameter downstream primary breakup is triggered and intensifies  
 453 farther downstream. Up to 5 diameters from nozzle exit, the core breakup process is fully developed since  
 454 the liquid core is narrowing to tapered ligaments. The liquid core is totally disintegrated at 8 diameters  
 455 downstream, resulting in higher numbers of droplets than at the positions upstream.

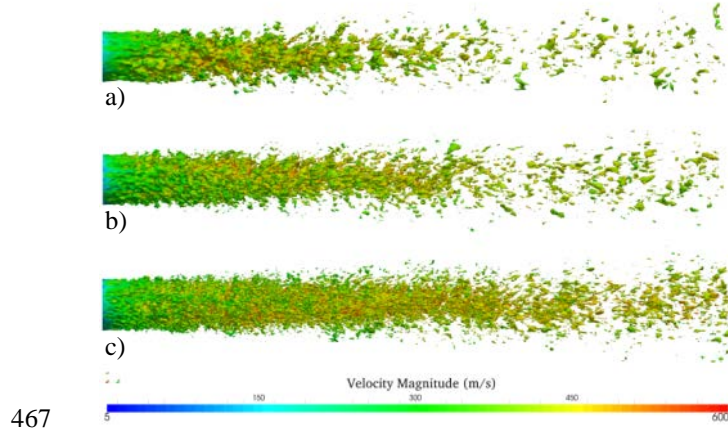




**Figure 14.** Liquid distribution in cross-sectional planes at different streamwise positions downstream of the nozzle exit for the coarse (left column), medium (middle column) and fine (right column) cases at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar). The value of  $z/D$  indicates the number of nozzle diameters downstream of the nozzle exit.

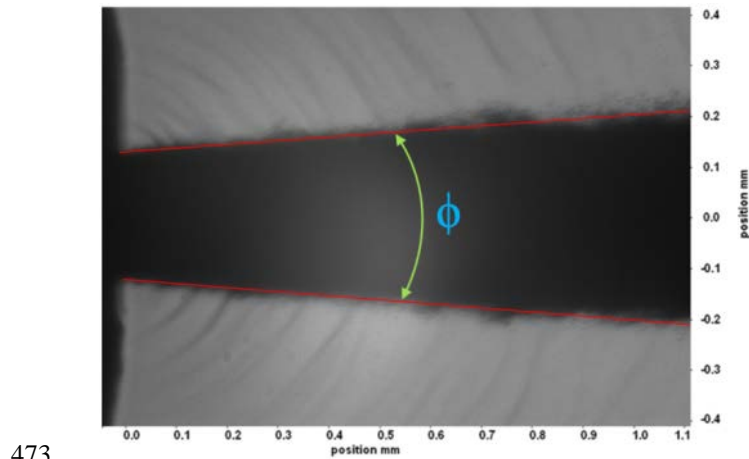
Figure 15 illustrates the liquid core visualized using the  $\gamma = 0.95$  isosurface at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar) for different meshes. It can be seen that longitudinal surface perturbations develop near the nozzle exit. The liquid core tapers progressively before disintegrating into large clusters which is in accordance with the limited available data by [51]. The fine mesh case shows an extended liquid core

465 compared to the coarser cases. This is due to pinching-off of smaller droplets from thinner ligaments  
 466 detached from the liquid jet surface which slows down the liquid core disintegration process [8, 48, 49].



468 **Figure 15.** Effect of mesh resolution on jet liquid core length depicted by  $\gamma = 0.95$  isosurface for  
 469 a) Coarse, b) Medium and c) Fine mesh cases at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar).

470 Figure 16 depicts the early spray angle ( $\phi$ ) at quasi-steady stage, measured on a spray image using  
 471 edge detection based on a threshold filter. The formation and development of shear layer instabilities can  
 472 be clearly seen. The nozzle tip is apparent on the left side of the image.

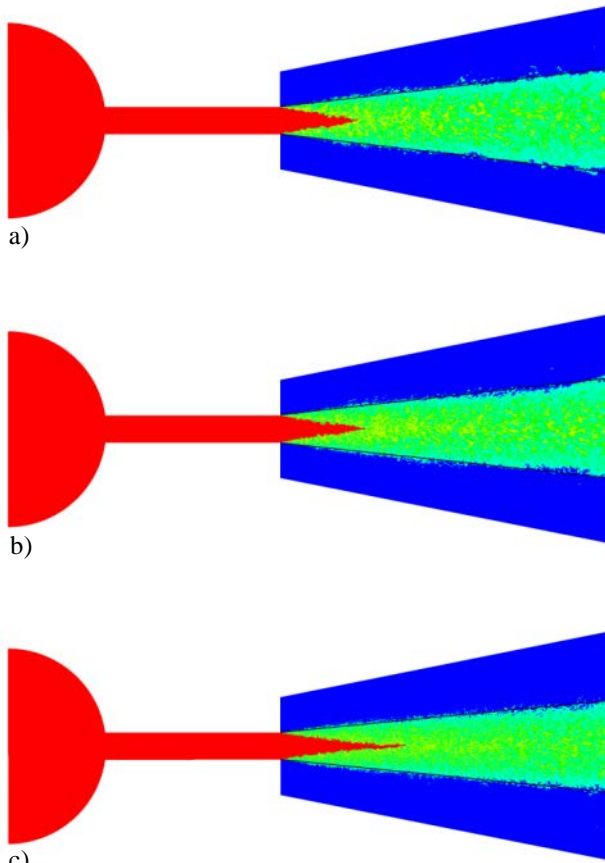


474 **Figure 16.** Shadowgraphy of the diesel nozzle spray at quasi-steady stage ( $P_{\text{inlet}} = 1200$  bar), using long  
 475 distance microscope[45].

476 To compare the predicted numerical early spray angle with experiment, Leboissetier & Zaleski [52]  
 477 core analysis was conducted. Based on this method, three different zones in the numerical data were



distinguished at every time step during the quasi-steady stage. The results of this analysis for three different cases are depicted in Figure 17, showing the time-averaged structure of the atomization region. The red zone contains only liquid (never contains gas), thus representing the liquid core; the blue region is gas only while the green region contains sporadic liquid and gas volumes depicting the atomization zone. The early spray angle was extracted using the outer boundary of the two phase mixture (green) zone.



**Figure 17.** A Leboissetier & Zaleski [52] core analysis for, a) Corase, b) Medium, and c) Fine at quasi-steady stage,  $P_{inlet}=1200$  bar; red and blue region experienced only liquid and gas, respectively. The green zone is the atomization region.

A summary of this investigation, gathered using these plots (Figure 17) is tabulated in Table 4, showing the reduction in spray angle and increase in liquid core length for the higher mesh resolution cases. For comparison, the core length predicted by Hiroyasu and Arai's correlation [17] is also shown.

The predicted core length appears to be too small and this may be partly due to the methods used to determine core length and partly due to the absence of a cavitation model, and thus overly high jet turbulence.

**Table 4.** Comparison of spray angle and liquid core length

Case	Early Spray Angle	Core Length (mm)
Experiment	$8.7 \pm 0.4^\circ$	-
Coarse	$13.22 \pm 1^\circ$	$0.71 \pm 0.05$
Medium	$12.52 \pm 0.8^\circ$	$0.73 \pm 0.05$
Fine	$11.26 \pm 0.5^\circ$	$1.151 \pm 0.02$
Hiroyasu & Arai [17]		9.13

#### 4. Conclusions

The general structure of primary atomization of diesel sprays was successfully characterized numerically employing an Eulerian/LES/VOF approach to capture free surfaces. The umbrella-shaped leading edge of the emerging jet was captured successfully near the nozzle exit. The experimental shadowgraphy images showed a rougher surface, greater transparency, more oblique angle and earlier disintegration of the leading edge in comparison with the numerical prediction. This is presumed due to in-nozzle air inclusions left from the previous injection event. The necking of the liquid jet behind the umbrella-shaped leading edge is captured in both experimental and numerical results. The temporal variation of jet penetration velocity and Reynolds number show favorable agreement between numerical and experimental results. The second-order temporal integration scheme and NV Gamma convection-specific interpolation scheme resulted in a better prediction of small scale eddies and jet surface structures compared with the first-order integration scheme and TVD convection-specific interpolation schemes.

A mesh resolution study for the two stages of the spray, initial penetration and quasi-steady, revealed that:

- fragmentation of the jet commenced close to nozzle exit (within about one diameter from exit) for the finest mesh
- modelling of the primary breakup process is enhanced with higher mesh resolution
- droplet sizes decrease with increasing mesh resolution
- smaller eddies were captured with decreasing cell size inside the nozzle
- increasing mesh resolution leads to decrease in the early spray angle and increase in the liquid core length, leading to better agreement between experiment and numerical predictions.

## Acknowledgments

This work was supported by the Australian Maritime College and the Defence Science and Technology Group. The authors express their gratitude to colleagues Luciano Mason, Jalal Rafie Shahraki for their support and suggestions. The authors also express gratitude to Hongjiang Yu for his assistance with the analysis of drop sizes..

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